# THERMODYNAMICAL PREDICTIONS OF NANODIAMONDS SYNTHESIZED BY PULSED LASER ABLATION IN LIQUID

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**Keywords**: nanodiamond, thermodynamics, nucleation, Gibbs free energy, stability

## Abstract

3-5 nm ultrananocrystalline diamonds have emerged as potentially revolution materials for various applications. As with all nanomaterials, the nanodiamond synthesis has a large impact on the usefulness of these materials. For instance, control of the size of nanodiamonds and a high transition probability from graphite to diamond has been pursued in nanodiamonds syntheses both theoretically and experimentally in recent years. Recently, a novel method of pulsed- laser ablation in liquid, so-called pulsed-laser induced liquid-solid interfacial reaction (PLIIR), has been intensively studied aimed at the synthesis of the metastable nanocrystals. By using PLIIR, a series of nanocrystals including diamond with cubic and hexagonal structure, cubic $C_3N_4$, and boron nitride with cubic and other metastable structures were prepared. More recently, PLIIR was extended to synthesize metastable one-dimensional nanostructures and ultrananocrystals. Accordingly, PLIIR is expected to be advantageous in the preparation of metastable nanocrystals that prefer a state of high pressure and high temperature. More importantly, PLIIR is a relatively new laser-based material processing method, and the mechanisms involved in the nucleation and phase transition of nanocrystals upon PLIIR are not well understood. It is therefore important to provide theoretical tools to investigate the physical and chemical phenomena involved in this processing method. Based on the nanothermodynamical approach, we performed the thermodynamical predictions of nanodiamonds synthesized by pulsed laser ablation in liquid. The nanothermodynamical analyses showed that the formation of nanodiamonds with sizes of 3-5 nm would be preferable to that of large nanodiamonds in the pressure-temperature region of 10-15 GPa and 4000-5000 K created by pulsed laser ablation of a graphite target in water in the carbon phase diagram. Meanwhile, the probabilities of the phase transition from graphite to diamond are calculated to be rather high, up to $10^{-3}$-$10^{-2}$ in the same pressure-temperature region. These theoretical results indicated that pulsed laser ablation in liquid is expected to be an effective industrial route to synthesize ultrananocrystalline diamonds.